CLAIMS

What Is Claimed Is:

1. A crystal comprising LuxS in crystalline form.

2. The crystal of Claim 1 wherein the LuxS is *H. pylori* LuxS, *H. influenzae* LuxS or *D. radiodurans* LuxS.

3. The crystal of Claim 1 which is diffraction quality.

4. The crystal of Claim 1 which is a native crystal.

5. The crystal of Claim 1 which is a heavy-atom derivative crystal.

6. The crystal of Claim 1 in which LuxS is a mutant.

7. The crystal of Claim 6, in which the mutant is a selenomethionine or selenocysteine mutant.

8. The crystal of Claim 6, in which the mutant is a conservative mutant.

9. The crystal of Claim 6, in which the mutant is a truncated or extended mutant.

10. The crystal of Claim 1 which is characterized by a diffraction pattern that is substantially similar to the diffraction pattern of FIG. 2., FIG 3., FIG 4. or FIG 5.

11. The crystal of Claim 1, which is characterized by a unit cell of a=71.04±0.7Å, b=71.04±0.7Å, c=130.14±1.3Å, α =90.0, β =90.0, and γ =90.0.

12. The crystal of Claim 1, which is characterized by a unit cell of a=129.59±1.3Å, b=129.59±1.3Å, c=53.74±0.5Å, α =90.0, β =90.0, and γ =90.0.

13. The crystal of Claim 1, which is characterized by a unit cell of a=43.53±0.5Å, b=81.87±0.8Å, c=49.30±0.5Å, α =90.0, β =102.85, and γ =90.0.

14. The crystal of Claim 1, which is characterized by a unit cell of a=51.08±0.5Å, b=70.04±0.7Å, c=49.75±0.5Å, α =90.0, β =102.85, and γ =90.0.

15. The crystal of Claim 1, which is produced by a method comprising the steps of:

(a) mixing a volume of a solution comprising the LuxS with a volume of a reservoir solution comprising a precipitant; and

(b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization until the crystal forms.

16. The crystals of Claims 11-14, wherein the precipitant is present in a concentration between about 15% and about 35% (w/v).

17. The crystals of Claims 11-14 wherein the precipitant is polyethylene glycol or PEG MME with an average molecular weight between about 1000 Da and about 10000 Da.

18. The crystals of Claims 11-14, wherein the solution further comprises between about 10 mM and about 200 mM buffer.

19. The crystals of Claim 18 wherein the buffer is HEPES, Tris, MES, MOPS, Bis-Tris, Sodium cacodylate, ACES, ADA, BES, or Citric acid.

20. The crystals of Claims 11-14, wherein the solution further comprises between 0 mM and about 300 mM ammonium sulfate.

21. The crystals of Claims 11-14, wherein the solution has a pH of between about 5.0 and about 7.0.

22. The crystals of Claims 11-14, which is produced by incubating the mixture comprising LuxS and reservoir solution at a temperature of between about 4 °C and about 25°C.

23. A method of making the crystal of Claim 1, comprising:

(a) mixing a volume of a solution comprising a LuxS polypeptide with a volume of a reservoir solution comprising a precipitant; and

(b) incubating the mixture obtained in step (a) over the reservoir solution in a closed container, under conditions suitable for crystallization until the crystal forms.

24. The method of Claim 23 wherein the LuxS polypeptide is *H. pylori* LuxS polypeptide, *H. influenzae* LuxS polypeptide or *D. radiodurans* LuxS polypeptide.

25. The method of Claim 23, wherein the precipitant is PEG or PEG MME with an average molecular weight between about 1000 and about 10000.

26. The method of Claim 23, wherein the precipitant is present in a concentration between about 15 % and about 35 % (w/v).

27. The method of Claim 23, wherein the solution further comprises between about 10 mM to about 200 mM buffer.

28. The method of Claim 27 wherein the buffer is HEPES, Tris, MES, MOPS, Bis-Tris, Sodium cacodylate, ACES, ADA, BES, or Citric acid.

29. The method of Claim 23, wherein the solution further comprises between about 0 mM and about 300 mM ammonium sulfate.

30. The method of Claim 23, wherein the solution has a pH of between about 5.0 and about 7.0.

31. The method of Claim 23, wherein the mixture comprising LuxS and reservoir solution is incubated at a temperature of between about 4 °C and about 25 °C.

32. A machine-readable medium embedded with information that corresponds to a three-dimensional structural representation of a crystal comprising LuxS in crystalline form, or a fragment or portion thereof.

33. The machine readable medium of Claim 32, in which the LuxS is *H. pylori* LuxS, *H. influenzae* LuxS or *D. radiodurans* LuxS.

34. The machine readable medium of Claim 32, in which the crystal is diffraction quality.

35. The machine readable medium of Claim 32, in which the crystal is a native crystal.

36. The machine readable medium of Claim 32, in which the crystal is a heavy-atom derivative crystal.

37. The machine readable medium of Claim 32, in which the crystalline LuxS is a mutant.

38. The machine readable medium of Claim 37, in which the mutant is a selenomethionine or selenocysteine mutant.

39. The machine readable medium of Claim 37, in which the mutant is a conservative mutant.

40. The machine readable medium of Claim 37, in which the mutant is a truncated or extended mutant.

41. The machine-readable medium of Claim 32, in which the information comprises the atomic structure coordinates, or a subset thereof.

42. A machine-readable medium embedded with the atomic structure coordinates of Table 7, Table 8, Table 9, or Table 10, or a subset thereof.

43. A method of identifying a LuxS binding compound, comprising the step of using a three-dimensional structural representation of LuxS, or a fragment thereof comprising a LuxS substrate binding site, to computationally screen a candidate compound for an ability to bind the LuxS substrate binding site.

44. The method of Claim 43 further including the steps of:
synthesizing the candidate compound; and
screening the candidate compound for LuxS binding activity.

45. The method of Claim 43 in which the structural information comprises the atomic structure coordinates of residues comprising a LuxS substrate binding site.

46. The method of Claim 43 in which LuxS is *H. pylori* LuxS, *H. influenzae* LuxS or *D. radiodurans* LuxS.

47. A method of identifying a LuxS binding compound comprising the step of using a three-dimensional structural representation of LuxS, or a fragment thereof comprising a

LuxS substrate binding site, to computationally design a synthesizable candidate compound that binds LuxS.

48. The method of Claim 47 in which the computational design comprises the steps of:

identifying chemical entities or fragments capable of associating with the LuxS substrate binding site; and

assembling the chemical entities or fragments into a single molecule to provide the structure of the candidate compound.

49. The method of Claim 48 further including the steps of:

synthesizing the candidate compound; and

screening the candidate compound for LuxS binding activity.

50. The method of Claim 48 in which the structural information comprises the atomic structure coordinates of residues comprising a LuxS substrate binding site.

51. The method of Claim 48 in which the LuxS is *H. pylori* LuxS, *H. influenzae* LuxS or *D. radiodurans* LuxS.

52. A method of designing a mutant LuxS comprising the steps of:

identifying a functional amino acid residue in the primary sequence of a three-dimensional representation of a LuxS molecule produced with the machine readable medium of Claim 32; and

altering the functional amino acid residue in the primary sequence of the LuxS molecule.

53. A method of preparing a mutant LuxS comprising:

desinging a mutant LuxS according to Claim 52; and

synthesizing the mutant LuxS.